Core-Level X-Ray Standing Wave Measurements on the Perovskite $La_{1/2}Sr_{3/2}MnO_4$

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Beamline(s): **X24A**

We examine the bulk atomic structure of the perovskite $La_{1/2}Sr_{3/2}MnO_4$ using photoemission-yield X-ray standing waves.

The perovskite structure is common to colossal magnetoresistive (manganite) and high-T_C superconducting (cuprate) materials. The origin of these effects are the Mn-O (or Cu-O) planes in the layered planar tetragonal structure of the perovskites, and "charge ordering" and "orbital ordering" of valence electrons in the Mn-O plane have been seen at low temperatures. In addition, dopants are added to provide additional charge carriers and tune the properties of the materials. In $La_{1/2}Sr_{3/2}MnO_4$, La replaces Sr as a dopant.

Core-level X-ray standing waves (XSW) has the advantage over X-ray diffraction that it is element specific. The atomic position distribution of each of the four elements in $La_{1/2}Sr_{3/2}MnO_4$, can be separated.

Experiments were performed at Beamline X24A at the NSLS. The $La_{1/2}Sr_{3/2}MnO_4$ sample was cleaved in ultrahigh vacuum (10^{-10} torr) to expose the (001) surface. Five reflections – (006), (114), (116), (204), and (213) – were examined in the backreflection configuration, at Bragg energies of $h\nu$ = 2987.6 eV, 3017.3 eV, 3750.1 eV, 3773.8 eV, and 3882.6 eV, respectively. The increased angular width of Bragg reflections in backreflection accommodates the mosaicity of the sample. The monochrometer crystals were Si(111).

Core-level yields were monitored by defining the hemispherical analyzer energy window around the core-level peak. A sample bias is applied to keep the photoemission peak centered in the window as the photon energy is swept through the Bragg condition. Background yields were collected using a second energy window at binding energies just below the peak, and were subtracted from the on-peak yields.

Figures 1 and 2 show the (006) and (204) photoemission XSW yields, respectively, of La, Sr, Mn, and O core-levels. For the (006) reflection, all four yields have a lineshape corresponding to a coherent position of zero, indicating that the position distribution of each element is centered on the diffraction plane. For the (204) reflection, the La and Sr yields again have a lineshape with a coherent position of zero, while Mn and O have lineshapes indicating coherent positions of 1/2. The other three reflections – (114), (116), and (213) – single out the Mn, in-plane O, and out-of-plane O atoms, respectively, placing them at a coherent position of 1/2 while the remaining atoms are at a position of zero. This contrast between the yields directly indicates the differences in the position distributions of each element in $La_{1/2}Sr_{3/2}MnO_4$.

The size of the features, which corresponds to the coherent fraction or amplitude of the XSW structure factor, is largest for Mn, intermediate for O, and smallest for La and Sr in Figure 1. This agrees with the known perovskite structure in that the Mn atoms and half of the O atoms are in crystallographic positions on the Mn-O planes, while the La, Sr, and other half of O atoms are distributed about the diffracting planes at distances which are not integer or half-integer multiples of the diffraction plane spacing. Note the small feature size of the O 1s yield of Figure 2. For the (204) reflection, the XSW contribution of half of the O atoms outside the Mn-O planes cancels that of the in-plane O atoms, for a total coherent fraction near zero.

The XSW data for all five reflections are consistent with the perovskite structure and lattice parameters determined from X-ray diffraction. In addition, for all five reflections, the La and Sr core-level yields produced the same lineshape and feature size. This is a direct verification that La substitutes exactly in the Sr sites, without distortion due to the difference in the atomic sizes of La and Sr.

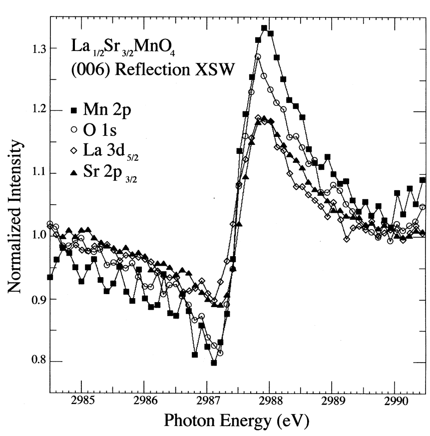

Figure 1. Mn 2p, O 1s, La $3d_{5/2}$, and Sr $2p_{3/2}$ core-level photoemission XSW yields as a function of photon energy for the (006) backreflection of $La_{1/2}Sr_{3/2}MnO_4$.

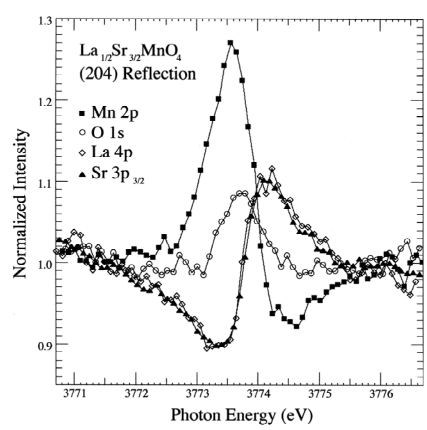

Figure 2. Mn 2p, O 1s, La 4p, and Sr $3p_{3/2}$ core-level photoemission XSW yields as a function of photon energy for the (204) backreflection of $La_{1/2}Sr_{3/2}MnO_4$.